On the Problem of Predicting Inflationary Perturbations

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Abstract

We examine the theoretical foundations of standard methods for computing density perturbations in inflationary models. We find that: (1) the time-delay formalism (introduced by Guth and Pi, 1982) is only valid when inflation is well-described by the de Sitter solution and the equation-of-state is nearly unchanging; and, (2) the horizon-crossing/Bessel approximation extends to non-exponential inflation, but only if the equation-of-state is changing slowly. Integration of the gauge-invariant perturbation equations mode-by-mode is the only method reliable for general models. For models with rapidly varying equation-of-state, the correction leads to significantly different predictions for the microwave background anisotropy. An important corollary is that methods proposed for "reconstruction" of the inflaton potential from anisotropy data are unreliable for general models.

One of the most important predictions of inflationary cosmology[1−3] is that quantum fluctuations of the inflaton field grow into cosmological energy-density perturbations.[4−8]. In this paper, we analyze and compare the standard methods for computing perturbation spectra in inflation. This consideration is motivated by the need to have theoretical predictions which match the precision anticipated in forthcoming measurements. We find that the simplest, most commonly used methods are approximations with narrow ranges of validity. The only reliable method for general potentials is the gauge invariant method[5,9,10] in which the equation-of-motion for the perturbation must be integrated for each mode.

The paper has several disparate components which we have organized by section for the convenience of the reader: (1) a review of the "exact" gauge invariant methods[5,9,10] with attention to some subtleties which have caused confusion in past literature; (2) an analysis of the time-delay formalism demonstrating that it is valid only when inflation is nearly de Sitter (exponential inflation); (3) an analysis of the horizon-crossing/Bessel function approach,[5,8,7,11] which show that it extends to non-exponential inflation but only if the equation-of-state is changing slowly; (4) example (Figure 1) of how the approximate methods can lead to large errors in computation of cosmic microwave background (CMB) anisotropy in cases of rapidly varying equation-of-state; (5) a summary in terms of conditions on the inflaton potential for applying the time-delay and horizon-crossing approximations and discussion of implications for "reconstructing" the inflaton potential and constraining cosmological parameters from (CMB) anisotropy and large-scale structure data.

Exact Method:[5,9,10] In this paper, we consider the case of a single inflaton field; multi-field inflation introduces other subtleties that we will discuss in a future paper.[12] The most general form for the metric with linear scalar perturbations is[13,14]:

$$ds^2 = a^2(\tau)\{(1+2\phi)d\tau^2 - 2B_{|i}dx^i d\tau - [(1-2\psi)\delta_{ij} + 2E_{|ij}]dx^i dx^j\} \tag{1}$$

where ϕ, B, ψ and E are arbitrary functions of space and time. A gauge-invariant combination of these variables is the gravitational potential,

$$\Phi = \phi + \frac{1}{a}[(B - E')a]', \tag{2}$$

where prime means derivative with respect to conformal time τ. The potential Φ is simply related to the anisotropy of the CMB on large angular scales via

$$\frac{\delta T}{T} \simeq \frac{1}{3}\Phi. \tag{3}$$

However, Φ is not the most convenient variable for tracing the generation of perturbations by quantum fluctuations. For this purpose, it is useful to introduce a second gauge invariant quantity[10]

$$v \equiv a\left(\delta\varphi + \frac{z}{a}\psi\right) \tag{4}$$

where $\delta\varphi$ is the perturbation in the scalar inflaton field: $\varphi_{total}(\vec{r},t) = \varphi_0(t) + \delta\varphi(\vec{r},t)$. During inflation, the variable z is

$$z \equiv a\sqrt{\epsilon} \tag{5}$$

where ϵ is the variable that characterizes the equation-of-state:

$$\epsilon = \frac{3}{2}\left(\frac{\rho + p}{\rho}\right); \tag{6}$$

for an inflaton with potential $V(\varphi)$, pressure $p = \frac{1}{2}\dot{\varphi}^2 - V(\varphi)$, and energy density $\rho = \frac{1}{2}\dot{\varphi}^2 + V(\varphi)$. Hence, $z = a\dot{\varphi}/H$, where $H = \dot{a}/a = a'/a^2$ is the Hubble constant and dot denotes the derivative with respect to the physical time $t = \int a d\tau$. We use everywhere the units where $4\pi G = 1$. In the post-inflationary phase when the universe is filled with hydrodynamical matter, the definition of z in Eq. (5) is replaced by $z = (a/c_s)\sqrt{\epsilon}$ where c_s is the speed of sound and, in the definition for v in Eq. (4), $\delta\varphi$ is replaced by the potential of the peculiar velocities in the matter.

By expanding $v(x,\tau)$ in Fourier modes with comoving wavenumbers k, the equation -of-motion for Fourier component v_k becomes (after lengthy computation):

$$v_k'' + \left(k^2 - \frac{z''}{z}\right) v_k = 0 \tag{7}$$

(k^2 is replaced by $c_s^2 k^2$ in the post-inflationary stage). The canonical variable v used in deriving quantum fluctuations beginning from an action describing the scalar field coupled to Einstein gravity;[10] and, it can also be simply related to the gravitational potential Φ via the constraint equation derived from the $0-0$ component of the Einstein equations:

$$\Phi_k = -\frac{H}{k^2 a} z^2 \left(\frac{v_k}{z}\right)' \tag{8}$$

The rigorous method to compute the perturbation spectrum is to solve the second order equation for each v_k using Eq. 7, beginning from when the given wavelength is small compared to the horizon to when it grows much larger than the horizon. To characterize the perturbations we use the power spectrum of $\zeta = v/z$ defined as:

$$P_\zeta(k) = \frac{k^3}{2\pi^2} \left|\frac{v_k}{z}\right|^2, \tag{9}$$

This power spectrum can be easily related with the power spectrum of the gravitational potential if we use Eq. (8), assuming z does not vanish. Note that all of the equations above describe the perturbations not only during inflation, but also in the post-inflationary (hydrodynamical) Universe. After inflation, $\epsilon = \mathcal{O}(1)$ and for the long wavelengths perturbations ($c_s^2 k^2 << |z''/z|$), $\Phi_k \sim \mathcal{O}(1)\zeta_k$. Hence, P_ζ is, up to a constant of order unity, the power spectrum of the gravitational potential that is of interest for computing perturbations of the CMB and the formation of large-scale structure. In this paper, our focus is on the fluctuations in ζ and their sensitivity to the equation-of-state, ϵ, during the inflationary epoch.

We note that some discussions of the exact approach improperly characterize ζ as a "conserved quantity." Indeed, an approximate conservation law can be derived for ζ using Eq. (8) and taking the long-wavelength limit $k \to 0$. However the "conservation law" is not strictly true for finite k and neglecting that fact can lead to some confusion.[15] For example, integrating the equation,

$$\frac{v}{z} \equiv \zeta = \frac{\Phi'/\mathcal{H} + \Phi}{\epsilon} + \Phi, \tag{10}$$

which follows from $0 - i$ Einstein equations, one can obtain Φ for a given ζ; in the long-wavelength limit (*i.e.,* to lowest order in k), one appears to obtain non-physical, extra constants of integration. To see that there are not additional integration constants, one should use constraint equation Eq. (8) and keep terms to order k^2. The "extra" constants are then fixed in terms of the "old" ones.

Time-delay Formalism: The time-delay formalism[6] is one of the methods originally introduced to compute the energy density perturbation spectrum at the end of inflation. In this method, the perturbations are related to the proper time delay $\delta\tau(x)$ between when inflation ends at position x compared to the spatial average. Here, we wish to show that this method is limited to cases in which the inflaton potential can be treated as nearly flat. To be sure, the time-delay formalism is a more intuitive derivation than the gauge-invariant approach and treating the potential as flat suffices as a crude estimate for some models. However, if one is interested in a rigorous treatment or more general models, including typical models of chaotic, natural, and power-law inflation, the time-delay formalism fails.

The time-delay method was originally presented for a toy model in which the inflationary phase is well-described by the de Sitter solution terminated by an instantaneous transition to a hydrodynamical stage. The aspects of the toy model which are essential to the time-delay approach are: (a) the metric perturbations can be completely ignored during the strictly de Sitter stage, and (b) the time delay for the perturbations with comoving wave number k, defined as $\delta\tau_k = \delta\varphi_k(t)/\dot{\varphi}_0(t)$, approaches a time-independent constant when the perturbation stretches well beyond the horizon.

Formally, the time-delay formalism cannot be made rigorous for any model, as it follow from the equation for the background $\dot{H} = -\dot{\varphi}_0^2$. The strict de Sitter limit, $\dot{H} = 0$, requires that $\dot{\varphi}_0 = 0$, in which case $\delta\tau_k = \delta\varphi_k(t)/\dot{\varphi}_0(t)$ is divergent. However, there is a limited range of models for which the formalism gives the leading order contribution. This range is

what we wish to clarify here. If one assumes the slow-roll approximation in which $\ddot{\varphi}$ can be ignored in the equation-of-motion for φ, then

$$\dot{\varphi}_0 \approx -V_{,\varphi}/3H, \tag{11}$$

where $V_{,\varphi} = dV/d\varphi$. The perturbation $\delta\phi$, satisfies the perturbed, linearized Klein-Gordon equation:

$$\delta\ddot{\varphi} + 3H\delta\dot{\varphi} - \frac{1}{a^2}\nabla^2\left(\delta\varphi + a\dot{\varphi}_0(B - a\dot{E})\right) + V_{,\varphi\varphi}\,\delta\varphi + 2V_{,\varphi}\,\phi - \dot{\varphi}_0(\dot{\phi} + 3\dot{\psi}) = 0, \tag{12}$$

which is supplemented by the $0 - i$ Einstein equation

$$\dot{\psi} + H\phi = \dot{\varphi}_0\delta\varphi. \tag{13}$$

In the long-wavelength and slow-roll limits, $\ddot{\varphi}$ and time- and spatial-derivatives of the metric parameters can be dropped:

$$3H\delta\dot{\varphi} + \left(V_{,\varphi\varphi} - \frac{(V_{,\varphi})^2}{V}\right)\delta\varphi = 0. \tag{14}$$

(In dropping these terms, we ignore the decaying modes and assume a generic gauge in which none of the variables characterizing the perturbations are suppressed compared to others by the gauge choice.) The solution for $\delta\varphi$

$$\delta\phi = C\frac{V_{,\varphi}}{V}, \tag{15}$$

where the constant $C \equiv (HV_{,\varphi}/V)_0$ can be expressed in terms of V and H evaluated at horizon-crossing for the given mode; this choice of C guarantees that $\delta\varphi \to H$ at horizon-crossing as expected in the de Sitter limit.

The key point is that, from Eqs. (11) and (15), we find that

$$\delta\tau = \frac{\delta\varphi}{\dot{\varphi}_0} = \frac{1}{3}C\frac{H}{V} \propto \frac{1}{\sqrt{V}}. \tag{16}$$

Unless V is independent of $\varphi_0(t)$, $\delta\tau$ depends on time which is inconsistent with an essential criterion of the time-delay formalism. Since V is always φ-dependent in practice, the time-delay formalism is, at best, a lowest order approximation. Even so, it should only be applied

if the V is extremely flat and H is nearly constant over the range of e-folds of physical interest, typically the last 60 e-folds of inflation. If H is nearly constant over the 60-folds, then the integral of $\epsilon = d(1/H)/dt$ over the last 60 e-folds must be much less than $1/H$; if the integral is to be less by a factor $\delta \ll 1$, then we require

$$\begin{aligned} \epsilon &\leq \tfrac{\delta}{60}, \\ \tfrac{d\ln\epsilon}{dN} &\leq \tfrac{\delta}{60}, \\ \epsilon\tfrac{d\ln\epsilon}{dN} &\leq \tfrac{\delta}{3600}; \; \ldots \end{aligned} \tag{17}$$

where ϵ must satisfy these constraints during the last 60 e-folds, N is the number of e-folds, and ... refers to analogous constraints on higher order derivatives. This represents a narrow set of models which excludes common power-law and chaotic inflationary models.

Horizon-crossing/Bessel Approximation: The horizon-crossing/Bessel approximation is based on the exact gauge invariant method but circumvents mode-by-mode integration. A recent review[16] discusses prior work and contains references. The perturbation amplitude for a given mode as it enters the horizon in the post-inflationary epoch is expressed in terms of the amplitude when the mode crosses beyond the horizon during inflation. To obtain the latter amplitude, the solution of Eq. (7) for the non-decaying mode in the long-wavelength limit, $k^2 \ll |z''/z|$,

$$v_k \longrightarrow C(k)z \tag{18}$$

is matched to the solution in the short wavelength limit, $k^2 \gg |z''/z|$,

$$v_k \longrightarrow \frac{1}{\sqrt{2k}} e^{-ik\tau}. \tag{19}$$

at horizon-crossing, $k = \mathcal{O}(1)aH$. (The normalization in Eq. (19) follows from the fact that v is the quantum canonical variable and $c_s = 1$.) The matching condition determines $C(k)$; namely, $|C(k)| = \mathcal{O}(1)/\sqrt{2k}z$ where $z \equiv a\dot{\varphi}/H$ evaluated when $k = \mathcal{O}(1)aH$; hence, the power spectrum is

$$P_\zeta(k) \to \frac{k^3}{2\pi^2}|C(k)|^2 = \left(\frac{H^4}{\dot{\varphi}^2}\right)_0 \times \mathcal{O}(1) \tag{20}$$

in the long-wavelength limit, where the subscript 0 means that H and $\dot{\varphi}$ are evaluated at $k = aH$ precisely. The $\mathcal{O}(1)$ ambiguity reflects the fact that the actual matching condition is not so precise.

The Bessel approximation is an improvement of the horizon-crossing approximation intended to resolve the ambiguity by replacing simple matching at $k \sim aH$ with a Bessel function approximant to Eq. (7) valid in a range of wavelengths around $k^2 = |z''/z|$ and then matching this solution to the long- and short-wavelength limits. More accurately capturing the behavior of the exact solution near $k^2 = |z''/z|$ is important to our purpose because it is the integration of Eq. (7) over this wavelength regime that is sensitive to the time-variation of the equation-of-state, $\epsilon(t)$. Hence, the Bessel approximation not only replaces the $\mathcal{O}(1)$ in Eq. (20) with a known function, but specifically a function of ϵ.

The horizon-crossing/Bessel approximation appears at first glance to be a leading order expression in a systematic expansion that can be extended to arbitrarily high accuracy. Here we show that, in actuality, it is obtained by matching long-, intermediate- and short-wavelength solutions. In particular, the horizon-crossing/Bessel approximation assumes that the amplitude of a mode is determined by a conditions within a small range of e-folds around horizon-crossing for the given mode. If the equation-of-state is changing rapidly, this assumption breaks down.

The ratio z''/z in Eq. (7) can be re-expressed in terms of ϵ:

$$\frac{z''}{z} = 2H^2a^2\left(1 - \frac{\epsilon}{2} - \frac{3}{4}\frac{d\ln\epsilon}{dN} + \frac{1}{4}\epsilon\frac{d\ln\epsilon}{dN} + \frac{1}{8}\left(\frac{d\ln\epsilon}{dN}\right)^2 + \frac{1}{4}\frac{d^2\ln\epsilon}{dN^2}\right), \tag{21}$$

where $0 < \epsilon(N) < 1$ during inflation. Here the conformal time variable τ has been replaced with N, the remaining number of e-folds until the end of inflation: the differential dN satisfies $dN = -aHd\tau$. In Eq. (7), the cross-over between short-wavelength and long-wavelength behavior occurs at $k^2 \sim |z''/z|$. Note that this corresponds to horizon-crossing, $k \sim aH$, only provided that $\epsilon(N)$ does not change too rapidly, *e.g.,* $(d\ln\epsilon/dN,\, d^2\ln\epsilon/dN^2) \leq \mathcal{O}(1)$). This is a necessary but insufficient condition for the horizon-crossing approximation to be

valid.

Assuming this condition is satisfied, the solution to Eq. (7) for a given mode k can be expressed as a Bessel function about $k = aH$. To see this, it is useful to replace N with

$$x \equiv \ln(Ha/k) = \ln(\lambda_{ph}/H^{-1}) \tag{22}$$

where $\lambda_{ph} = a/k$ is the physical wavelength of the perturbation with comoving scale k. The variable x is roughly the number of e-folds after the given mode crosses the horizon during inflation; it is equal to zero at the moment of horizon-crossing, positive after horizon-crossing, and negative before horizon-crossing. Then, if we replace v with

$$\widetilde{v} = (1-\epsilon)^{1/2}(\exp(x/2))v \tag{23}$$

Eq. (7) takes the form

$$\frac{d^2\widetilde{v}}{dx^2} + \left[\frac{\exp(-2x)}{(1-\epsilon)^2} - \frac{1}{4}\left(\frac{3-\epsilon}{1-\epsilon}\right)^2 - \frac{3}{2}\frac{d\ln\varepsilon}{dx} + \frac{1}{2}\frac{d\ln(1-\epsilon)}{dx} - \frac{1}{4}\left(\frac{d\ln\epsilon(1-\epsilon)}{dx}\right)^2 - \frac{1}{2}\frac{d^2\ln\epsilon(1-\epsilon)}{dx^2}\right]\widetilde{v} = 0 \tag{24}$$

If $\epsilon =$ constant then this equation is reduced to a Bessel equation with exact solutions given by $\widetilde{v} \sim H_\nu^{(1,2)}\left(\frac{e^{-x}}{1-\epsilon}\right)$ where

$$\nu = \pm\frac{1}{2}\left(\frac{3-\epsilon}{1-\epsilon}\right) \tag{25}$$

However, $\epsilon =$ constant is not realistic for cosmology since the equation-of-state must change near the end of inflation in order to return to the ordinary, Friedmann-Robertson-Walker expansion rate. The standard approach has been to solve Eq. (24) approximately near the horizon crossing point $x = 0$ where

$$\epsilon(x) = \epsilon_0 + \epsilon_0\left(\frac{d\ln\epsilon}{dx}\right)_0 x + ... \tag{26}$$

The subscript 0 is used to symbolize horizon-crossing for the given mode, which is equivalent to evaluating at $x = 0$. The solution will be an approximation in which the small parameters are ϵ_0 and x -derivatives, $(d.../dx)_0$. More precisely, $\ln\epsilon_0$ is treated as a zeroth-order quantity; ϵ_0 and $(d\ln\epsilon/dx)_0-$ are first order quantities; ϵ_0^2, $\epsilon_0\,(d\ln\epsilon/dx)_0$, $(d\ln\epsilon/dx)_0^2$

and $(d^2 \ln \epsilon / dx^2)_0$ are second order quantities; etc. Note that $d \ln(1-\epsilon)/dx = -(\epsilon/(1-\epsilon))(d \ln \epsilon / dx)$ is second order.

Substituting (26) in Eq. (24), we obtain:

$$\frac{d^2 \widetilde{v}}{dx^2} + \left[\frac{\exp(-2x)}{(1-\epsilon_0)^2} - \frac{1}{4} \left(\frac{3-\epsilon_0}{1-\epsilon_0} \right)^2 - \frac{3}{2} \left(\frac{d \ln \epsilon}{dx} \right)_0 + R_2(x) \right] \widetilde{v} = 0 \tag{27}$$

where $R_2(x)$ denotes the second and higher order terms,

$$\begin{aligned} R_2 \; = \; & \left(\frac{1}{2} - \frac{2e^{-2x}}{(1-\epsilon_0)^2} x + \frac{3-\epsilon_0}{(1-\epsilon_0)^2} x \right) \left(\frac{d \ln(1-\epsilon)}{dx} \right)_0 \\ & - \frac{1}{4} \left(\frac{d \ln \epsilon}{dx} \right)_0^2 - \frac{1}{2} (1 + 3x) \left(\frac{d^2 \ln \epsilon}{dx^2} \right)_0 + O(\epsilon_0^3, ...) \end{aligned} \tag{28}$$

The initial conditions are fixed by the assumption that the short-wavelength behavior should be as in a flat Minkowski vacuum with only positive frequencies, resulting in the solution

$$\widetilde{v} = C_k H_\nu^{(1)}(\xi) \tag{29}$$

where $\xi \equiv \exp(-x)/(1-\epsilon_0)$, and

$$\nu = \frac{1}{2} \left(\left(\frac{3-\epsilon_0}{1-\epsilon_0} \right)^2 + 6 \left(\frac{d \ln \epsilon}{dx} \right)_0 - 4R_2 \right)^{1/2}, \tag{30}$$

provided we treat R_2 as constant – this is essential to using a Bessel function to represent the solution. However, R_2 is constant only in the case when $\epsilon =$ constant, in which case R_2 itself is precisely zero. The fact that ϵ and, hence, R_2 are x -dependent for realistic models is what imposes a limit on the validity of Bessel approximation and leads to the result that Bessel solution deviates more and more from the exact solution as $|x|$ grows. For example, it tells us that it is inappropriate to keep the terms smaller than R_2 in the expression for index ν. Consequently, keeping terms of order ϵ_0^2 in the expression for the index ν is invalid since these terms are comparable to or smaller than the contributions of the x -dependent terms in R_2 that have been neglected, unless R_2 vanishes. Eq. (30) should be re-expressed

$$\nu \simeq \frac{3}{2} + \epsilon_0 + \frac{1}{2} \left(\frac{d \ln \epsilon}{dx} \right)_0 + \delta_2 \nu. \tag{31}$$

where

$$\delta_2\nu \sim \frac{5}{4}\epsilon_0^2 - \frac{1}{3}R_2(x). \tag{32}$$

characterizes the "accuracy" with which the indexes in Bessel function solution should be trusted.

Our analysis illustrates a key limitation to the horizon-crossing and Bessel approximations: they cannot be improved further than first order by any reasonable scheme. We have just argued that extending the approximation to order ϵ_0^2 requires that we also keep the x-dependent terms in R_2; but then Eq. (30) is no longer solvable in terms in Bessel functions. Alternative schemes that we can imagine are as difficult as solving the exact equations, and, hence, have no advantage.

The error in ignoring $\delta_2\nu$ translates into an error in the Bessel approximation to the power spectrum that we wish to estimate. To obtain the spectrum, we extend the Bessel function approximant valid about $x = 0$ to the long-wavelength ($x \gg 0$ or $\xi \to 0$) limit:

$$H_\nu^{(1)}(\xi) = \frac{i\Gamma(\nu)}{\pi}\left(\frac{1}{2}\xi\right)^{-\nu}\left(1 - \frac{\xi^2}{4(1-\nu)} + O(\xi^3)\right) \tag{33}$$

and the short-wavelength ($x \ll 0$ or $\xi \to \infty$) limit:

$$H_\nu^{(1)}(\xi) = \sqrt{\frac{2}{\pi\xi}(P^2 + Q^2)}\exp\left(i\left(\xi - \frac{\pi\nu}{2} - \frac{\pi}{4} + arctg\left(\frac{Q}{P}\right)\right)\right) \tag{34}$$

where

$$\begin{aligned} P &= 1 - \tfrac{(4\nu^2-1)(4\nu^2-9)}{2!(8\xi)^2} + O(\tfrac{1}{\xi^4}) \\ Q &= \tfrac{4\nu^2-1}{8\xi} + O(\tfrac{1}{\xi^3}) \end{aligned} \tag{35}$$

Combining Eqs. (23), (31) and (33) and using $H = H_0(1 - \epsilon_0 x + \ldots)$, the extrapolation of the Bessel solution in the long-wavelength limit becomes

$$\begin{aligned} v = -iB_k\, z\,\sqrt{\frac{2}{\pi}}\frac{H_0}{k(\epsilon_0)^{1/2}}&\left(1 - \beta\epsilon_0 + \frac{1-\beta}{2}\left(\frac{d\ln\epsilon}{dx}\right)_0\right) \\ \times&\left(1 - \frac{\exp(-2x)}{4(1-\nu_0)(1-\epsilon_0)^2} + O(e^{-3x})\right)(1 + O(\delta_2\nu)) \end{aligned} \tag{36}$$

where $\beta = \ln 2 + \gamma - 1 = 0.27$ and γ is Euler's constant, and B_k is a constant to be determined by matching to the short-wavelength solution (to be discussed below). The last

term in Eq. (36) characterizes the deviation of the Bessel solution from the exact solution for v based on the exact equation, Eq. (24). This solution to the approximant (Bessel) equation is to be matched to the long-wavelength limit of the exact equation ($v = C(k)z$) to obtain $C(k)$ in terms of B_k, ϵ_0 and $(d\ln\epsilon/dx)_0$. We see that the match is best if x can be chosen so that the last two correction factors in parentheses in Eq. (36) are negligible compared to $\beta\,\epsilon_0$ and $\frac{1-\beta}{2}\,(d\ln\epsilon/dx)_0$. That requires that x be neither too small nor too big where the two solutions are matched. The first correction factor requires that the match-point $x = x_+$ satisfy $x_+ \geq max\,\left\{\left|\ln(\epsilon_0;\,\left(\frac{d\ln\epsilon}{dx}\right)_0\right|\right\}$, and the second factor requires that x_+ be sufficiently small that

$$\delta_2\nu(x_+) << \min(\epsilon_0;\left(\frac{d\ln\epsilon}{dx}\right)_0). \tag{37}$$

(Recall that $\delta_2\nu$ includes x-dependent terms that increase in magnitude with increasing x.) The result is that

$$x_+ \simeq \max\left\{\left|\ln\left[\min(\epsilon_0;\,\left(\frac{d\ln\epsilon}{dx}\right)_0\right]\right|\right\} \tag{38}$$

is optimal for obtaining the best match. The fact that the optimal match-point, x_+, is constrained from above and below means that there is a residual second-order error which cannot be improved upon by this matching procedure.

The matching of the Bessel solution to the short-wavelength limit proceeds similarly and determines B_k. Eq. (34) implies that

$$v = B_k\sqrt{\frac{2}{\pi}}\left(1 + O(1)\left(\frac{d\ln(1-\epsilon_0)}{dx}\right)_0 x + \frac{1}{2}\exp(2x) + O(e^{4x})\right)\exp(i(k\tau). \tag{39}$$

where the second terms inside the brackets comes as a result of uncertainty in Bessel function index, $\delta_2\nu$. This solution can be matched to the short-wavelength limit, $v \to \sqrt{1/2k}\,\exp(ik\tau)$ to first-order accuracy in ϵ_0 and $(d\ln\epsilon/dx)_0$ at match-point $x_- \simeq \frac{1}{2}\ln\left|\left(\frac{d\ln(1-\epsilon_0)}{dx}\right)_0\right|$, roughly two or so e-folds before the end of inflation for typical models. (Note that Eq. (39) contains two second-order correction terms, one of which increases with x and the other which

decreases with x. Consequently, just as with x_+, we find that the point x_-, the short-wavelength match-point which gives the best accuracy, is constrained from above and below.) The higher-order corrections are negligible provided

$$\delta_2 B(x_-) = O(1)\left(\frac{d\ln(1-\epsilon_0)}{dx}\right)_0 \ln\left|\left(\frac{d\ln(1-\epsilon_0)}{dx}\right)_0\right| \ll 1. \tag{40}$$

In this limit, $B_k = \sqrt{\pi/4k}(1+\mathcal{O}(1)\delta_2 B(x_-)$. Substituting this expression for B_k into the long-wavelength expression Eq. (36) and obtaining a complete first-order expression for $C(k)$, one can then determine the power spectrum:

$$P_\zeta(k) = \frac{k^3}{2\pi^2}\left|\frac{v_k}{z}\right|^2 = \left(\frac{H_0^4}{\dot\varphi}\right)_0 \frac{1}{4\pi^2}\left[1 - 2\beta\epsilon + (1-\beta)\left(\frac{d\ln\epsilon}{dx}\right) + O(1)\delta_2 B(x_-) + O(1)\delta_2\nu(x_+)\right]_0 \tag{41}$$

where the last two terms in square brackets characterize the uncertainty and should be smaller than the previous, first-order terms. Comparing to the original estimate, Eq. (20), we find that the $\mathcal{O}(1)$ factor has been replaced by a function which depends on the equation-of-state. The spectral index of the scalar power spectrum is then

$$n_s \equiv 1 + \frac{d\ln P_\zeta}{d\ln k} = \left(1 - 2\epsilon - \frac{d\ln\epsilon}{dx} - 2\epsilon^2 - 2\beta\epsilon\frac{d\ln\epsilon}{dx} + (1-\beta)\frac{d^2\ln\epsilon}{dx^2}\right)_0 + \ldots \tag{42}$$

and

$$\frac{dn_s}{dx} = (n_s - 1)\frac{d(n_s-1)}{dx} \tag{43}$$

$$= \left(-2\epsilon\frac{d\ln\epsilon}{dx} - \frac{d^2\ln\epsilon}{dx^2} - 4\epsilon^2\frac{d\ln\epsilon}{dx} - 2\beta\epsilon\left(\frac{d\ln\epsilon}{dx}\right)^2 - 2\beta\epsilon\frac{d^2\ln\epsilon}{dx^2} + (1-\beta)\frac{d^3\ln\epsilon}{dx^3}\right)_0 + \ldots \tag{44}$$

where $\ldots$ are uncertainty due to $\delta_2\nu$ and $\delta_2 B$. These expressions agree with previous results[16,17] except that they are expressed in terms of the equation-of-state and its derivatives.

Eqs. (37) through (41) summarizes the basic result: the Bessel approximation for $P_\zeta(k)$ is only good to first order in ϵ_0 and $(d\ln\epsilon_0/dx)_0$ *at best*, and then only if $\delta_2 B(x_-)$ and $\delta_2\nu(x_+)$ are negligible compared to the first order contributions. In previous discussions, it

was pointed out that the approximation was only valid if ϵ and $d\ln\epsilon/dx$ (or equivalents) are nearly constant over some range of e-folds around horizon-crossing,[16,17] but, otherwise, the conditions for the approximation to be valid were not specified. Here, we see that the relevant range of e-folds is between x_- and x_+ e-folds about $k = aH$, typically the five or so e-foldings surrounding horizon-crossing, $k = aH$. We also see that, as $x \to x_\pm$, the Bessel solution approaches the exact solution to within accuracy $\delta_2\nu$ and $\delta_2 B$; for x beyond this range, the Bessel approximant diverges from the true short- and long-wavelength solutions. Consequently, the Bessel approximant can achieve first order accuracy, but no better. Recall that we must also restrict ourselves to $d^2\ln\epsilon/dx^2 \leq \mathcal{O}(1)$ (see discussion under Eq. (21).

In special cases, a satisfactory numerical result can be obtained even though some constraints are not satisfied: A prominent example is natural inflation and other potentials of the form $V \approx V_0 - a\varphi^2 + \ldots$. In Eq. (38), two independent constraints are implied by the parenthetical $\left(\epsilon_0; \left(\frac{d\ln\epsilon}{dx}\right)_0\right)$. The first constraint ensures that the Bessel approximation gives the correct result to leading order in ϵ_0; the second ensures that the correct result to leading order in $\left(\frac{d\ln\epsilon}{dx}\right)_0$. For some natural inflation models, though, the first constraint is strongly violated so that the $\mathcal{O}(\epsilon_0)$ terms in the Bessel approximation cannot be "trusted." However, not only is the second constraint satisfied, but the terms in the Bessel approximation proportional to $(d\ln\epsilon/dx)_0$ are so much larger than the $\mathcal{O}(\epsilon_0)$ terms that the violation of the first constraint is numerically insignificant. The success of the Bessel approximation is accidental in this sense (and may have deceived some into thinking that the Bessel approximation has a much wider domain of validity than it actually does).

Our elaborate analysis can be reduced to a simple statement about domain of validity of the horizon-crossing/Bessel approximation:

(1) If $\epsilon =$ constant, any value in the inflationary range between 0 and 1, the Bessel solution is exact. However, a model with $\epsilon =$ constant is not physically realistic since inflation never terminates.

(2) If $\epsilon \neq$ constant, the Bessel approximation is only accurate if ϵ_0 and $(d\ln\epsilon/dx)_0$ are small enough that the first order contributions in ϵ_0 and $(d\ln\epsilon/dx)_0$ are much larger than the higher order contributions, $\delta_2\nu$ and $\delta_2 B$. Suppose we demand that the higher order terms on left-hand-side of Eq. (38) be less than a factor $\delta \ll 1$ times the first order terms on the right-hand-side of Eq. (38). (For example, δ might be determined by the resolution of an experiment and we may wish to know if the Bessel approximation provides the needed accuracy.) Assuming no accidental cancellations, Eqs. (37) through (40) reduce to:

$$\begin{aligned} \epsilon_0 &\leq \frac{\delta}{x_+} \\ \left(\frac{d\ln\epsilon}{dx}\right)_0 &\leq \frac{\delta}{x_+} \\ \left(\frac{d^2\ln\epsilon}{dx^2}\right)_0 &\leq \frac{2\epsilon_0\delta}{x_+} \leq \frac{\delta^2}{x_+^2};\ \ldots \end{aligned} \tag{45}$$

where $x_+ \equiv max \left\{ \left| \ln(\epsilon_0;\ \left(\frac{d\ln\epsilon}{dx}\right)_0 \right| \right\} > 1$ and $\ldots$ refers to analogous constraints on higher order derivatives. Even for modest accuracy, $\delta = 20\%$ and $x_+ \sim 2$, the ratio δ/x_+ is ~ 0.1, enough to highly restrict the range of ϵ and its derivatives.

Comparing the constraints above to Eq. (17), one sees that the horizon-crossing/Bessel approximation applies to a wider range of models than the time-delay formalism. Nevertheless, the range is narrow compared to full spectrum of inflationary models. One class of models in which the horizon-crossing/Bessel approximation is valid, where $(d\ln\epsilon/dx)_0 \ll \epsilon_0 \leq \delta/x_+ \ll 1$, includes the simplest models of new inflation[2,3,18], chaotic inflation[19] with ϕ^n potentials and $n >> 2$, and extended inflation[20,21], which are realistic models incorporating inflation. For these models, one obtains the CMB anisotropy prediction: n_s and r obey the relation[22]: $r \simeq 21(1+\gamma) \simeq 7(1-n_s)$, where $r \simeq \epsilon/14$ is the ratio of the tensor mode to the scalar mode in terms of the contribution to the CMB dipole moment. The second class, where $\epsilon_0 \ll (d\ln\epsilon/dx)_0 \ll \delta/x_+ \ll 1$, includes a range of natural inflation models,[23] chaotic inflation models with ϕ^n potentials and small n, and some two-field inflation models[24] in which the inflaton field rolls near an extremum of the potential during inflation.

Some may have assumed that the good agreement between the Bessel approximation and

the exact methods for these two cases meant that the Bessel approximation could be used for a broader range of models. In fact, our results show that these are essentially the only models for which the approximation can be trusted.

Impact on Microwave Background Anisotropy Prediction: An Illustration The error in using one of the approximate procedures instead of the more cumbersome mode-by-mode integration propagates to predictions of the cosmic microwave background anisotropy and large-scale structure. As a dramatic illustration, Figure 1 shows a comparison of the predicted CMB anisotropy power spectrum using the time-delay formalism or naive horizon-crossing approximation (based on Eq. (20)), the Bessel approximation (based on Eq. (41)), and the exact computation for a sample inflaton potential, $V(\phi) = \Lambda^4(1-\frac{2}{\pi}\, tan^{-1}(5\phi/m_p)$, in which the equation-of-state changes rapidly enough near $\phi = 0$ that Eq. (45) is not satisfied. (For this toy model, we have taken $\phi \approx -0.3$ to correspond to 60 e-folds before the end of inflation.) The discrepancy in the CMB predictions is large compared to the anticipated experimental resolution of future space-based anisotropy experiments. Less dramatic effects occur in more typical models with slowly varying equation-of-state; an analysis for a wide spectrum of models be presented in a future paper.[25]

Summary: Our conclusions are summarized in Eqs. (17) and (45) as constraints on the equation-of-state, ϵ. The basic result is that the time-delay and horizon-crossing methods are reliable approximations only if ϵ and its time-variation are rather small. These constraints can be re-formulated in terms of rules-of-thumb for an inflaton potential, $V(\varphi)$: Assuming higher-order corrections to our approximation should be $\delta < 0.20\%$ and $x_+ \approx 2$, then, if $V(\varphi)$ satisfies any of the following conditions (recall that $4\pi G = 1$ and $x_+ > 2$):

$$\left(\frac{V'}{V}\right)^2 \geq 4\frac{\delta}{x_+} \approx 0.4 \tag{46}$$

$$\frac{V''}{V} \geq \frac{\delta}{x_+} \approx 0.1 \tag{47}$$

$$\frac{V'V'''}{V^2} \geq \frac{\delta^2}{x_+^2} \approx 0.01 \tag{48}$$

during the last 60 e-folds of inflation, the horizon-crossing/Bessel approximation is not reliable and mode-by-mode integration is required. For the time-delay formalism, the constraints are roughly 60 times more stringent.

An important consequence is that attempts at precise fitting of CMB anisotropy data[26−27] and large-scale structure measurements and attempts to "reconstruct" the inflaton potential from CMB, as described in a recent review,[16] is not as straightforward as one hoped. If the horizon-crossing and reconstruction approaches were generally valid, then inflationary predictions could be parameterized with only a few variables (*e.g.*, ϵ_0 and $(d\ln\epsilon/dx)_0$ evaluated for the mode crossing the horizon in the present epoch). Simultaneous fitting of these parameters along with other cosmic parameters, (such as the Hubble constant, the cosmological constant, the baryon density, etc.) would provide tight constraints on all. Indeed, this approach has been assumed in most prior discussions of fitting data. To be sure, cases where the equation-of-state is nearly constant and the horizon-crossing approximation is valid appear to be the simplest forms of inflaton potential based on our current understanding. So, one can decide *a priori* to assume this subclass of inflationary potentials; in this case, there is no point to general reconstruction methods since the potential forms are set by the *a priori* assumption. Alternatively, one may make no *a priori* assumptions, in which case reconstruction methods are not useful since they are not valid for general potentials. If we broaden the spectrum of possible potentials, the fitting of cosmic parameters must be learned by comparing data to some systematic search through exact results obtained by mode-by-mode integration. How best to perform the search and how this affects the empirical resolution of cosmic parameters from CMB measurements is a subject of current investigation.[25]

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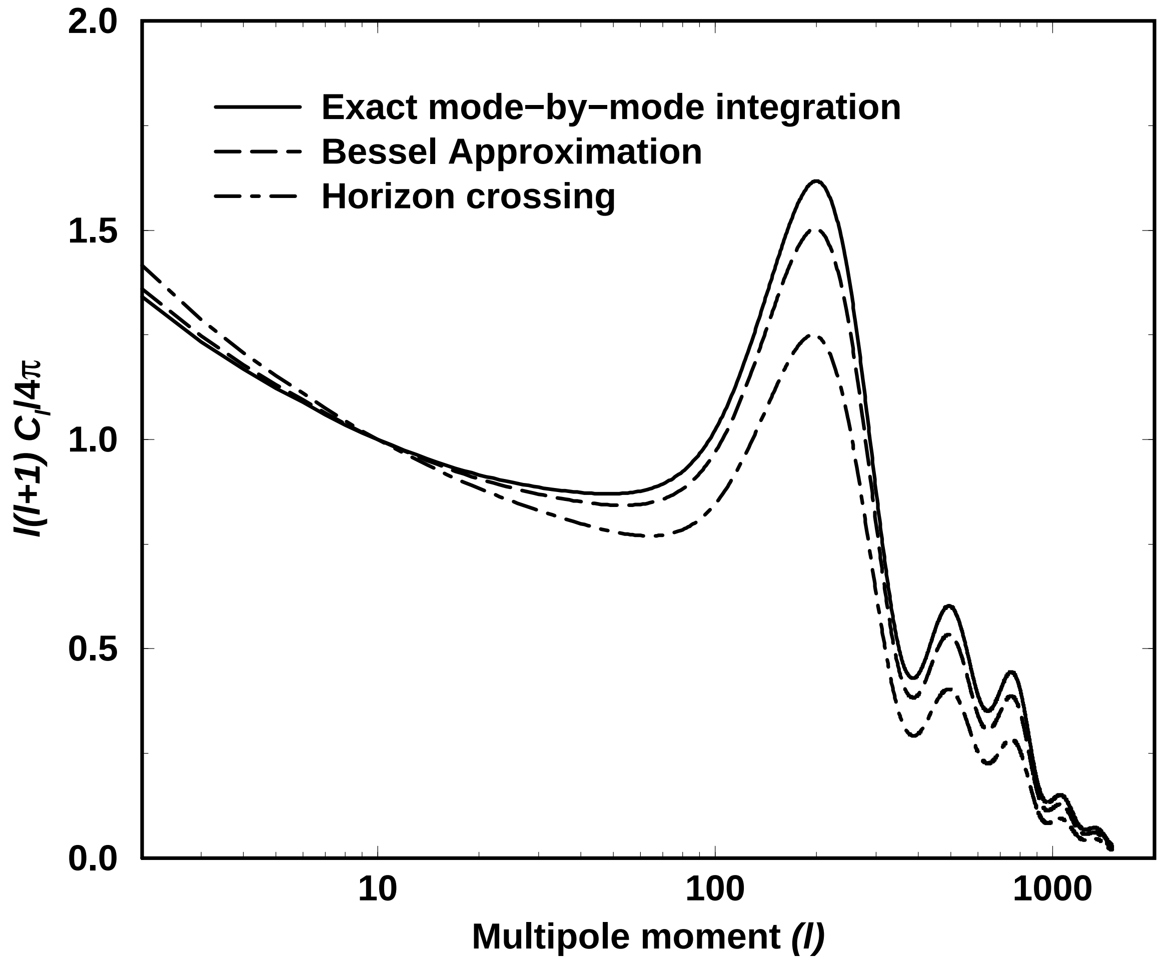

FIG. 1. A comparison of the horizon-crossing and Bessel approximations to exact mode-by-mode integration for an inflaton potential in which the equation-of-state (ϵ) is varying rapidly. The power spectrum has been computed and converted into a prediction of the CMB temperature anisotropy spectrum on large angular scales.